MM 69: Structural Materials (Steels, light-weight materials, high-temperature materials)

Structural Materials I

Time: Friday 9:30–10:45 Location: H 0106

MM 69.1 Fri 9:30 H 0106

Dislocation dissociations in C11b MoSi2 and their impact on its plastic deformation — Václav Paidar[1], Miroslav Čák[2], •Mojmír Šob[3,4,5], and Václav Vitek[6] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czechia — [2]ICAMS, Ruhr-Universität Bochum, Germany — [3]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czechia — [4]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czechia — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czechia — [6]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, U.S.A.

Using the DFT calculated γ-surfaces possible metastable stacking faults have been found for the most common slip planes {013} and {110} in MoSi2. These calculations reveal three distinct stacking faults on {013} planes and one stacking fault on {110} plane. Owing to such multiplicity of metastable stacking faults there is a large number of possible dislocation dissociations. These dislocation splittings are analysed using the anisotropic elasticity and relevant stacking faults. The results show that the only dissociations of the <331] dislocations favoured over the complete undissociated dislocations are on {013) planes either in one or two planes of this type. Splitting into {110) planes are never favored. For loading along the [001] axis the dislocation glide may take place at high temperatures when the cross slip releases the sessile screw dislocations on two {013) planes.

MM 69.2 Fri 9:45 H 0106

Evaluation of Fermi surfaces, single and two-particle spectral properties for FeSe using Quasi-particle self consistent GW + DMFT — •Swagata Acharya, Dimitar Pashov, and Mark van Schilfgaarde — King's College London, London, United Kingdom

Most of the first principles techniques, based on DFT or DFT+DMFT frameworks, fails to reproduce the spectral properties of the FeSe both in the tetragonal and orthorhombic phases. Within our recently developed quasi-particle self-consistent GW coupled to DMFT, we show how proper estimations of the non-local and local spin fluctuations reproduce the spectral properties in very good agreement with the experiments. We also compute the spin-wave excitation spectra and find momentum dependent shifts in spin-fluctuation weights across the structural transition at 90 K. We rigorously show how these compare with the extant experimental findings.

MM 69.3 Fri 10:00 H 0106

Chromium and iron based zeta phases - lattice dynamics from first-principles — •Petr Dvořáček and Dominik Legut — VSB Technical University of Ostrava

It was shown [1] that the Z-phase precipitates at higher rate in Cr-rich steels than in Cr-depleted ones and this precipitation correlates with the presence of Niobium. Recently, the lectronic structure and mechanical properties of Z-phases, namely CrNbN and CrVN, were investigated employing first-principles calculations [2]. In this contributions we extend our understanding for dynamical and thermodynamical properties of the Cr-(V/Nb/Mo)-N and Fe-(V/Nb/Mo)-N Z-phases based on the lattice vibrations computed within the quasi-harmonic approximations[3]. The requested Hellman-Feynman forces acting on atoms along the atomic vibrations were computed emlopying density functional theory via the Vienna Ab Initio Simulation package[4]. The results are following: CrNbN, CrVN, CrNbVN, FeNbN, FeNbVN are thermodynamically stable, CrMoN, FeVN are thermodynamically unstable, but are stable in gamma-point and FeMoN is completely thermodynamically unstable.

References: 1. H. K. Danielsen and J. Hald, Energy Mater. 1, 49 (2006). 2. D. Legut and J. Pavlů, J. Phys.: Condens. Matter. 24 , 195502 (2012). 3. A. Togo and I. Tanaka, Scr. Mater., 108, 1-5 (2015). 4. G. Kresse and J. Furthmueller, Comput. Mater. Sci. 6, 15 (1996).

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MM 69.4 Fri 10:15 H 0106

Theoretical and experimental investigation of mixing and clustering thermodynamics of Ti1-xAlxB2 alloys with age-hardening potential — •Erik Johansson, Nils Nedfors, Annop Ektarawong, Johanna Rosén, and Björn Alling — Linköping University - The Department of Physics, Chemistry and Biology (IFM)

Our project investigates phase stability and temperature dependence of structural parameters of Ti1-xAlxB2 metastable ceramic alloys. These alloys were predicted to exhibit a tendency for isostructural decomposition despite the fact that binary TiB2 and AlB2 are structurally very similar. Due to the reported high hardness of TiB2 and the prospect of age-hardening through isostructural clustering, these alloys could be good candidates for hard protective coatings on industrial cutting tools. In our work, we present theoretical predictions based on first-principles density functional theory. The phase diagram for this ternary system is derived and shows an isostructural miscibility gap. Phonon vibrational contributions to the free energies within harmonic and quasiharmonic approximations are calculated for the ordered binaries and disordered alloys, and we show their effect on the phase diagram. Non-isotropic thermal expansion beyond the standard implementation of the quasiharmonic approximation is investigated, and we discuss the methodological differences. Experimental synthesis of Ti1-xAlxB2 thin films using physical vapour deposition demonstrates the feasibility of growing the alloys, and after heat treatments at 1000 °C isostructural decomposition can be observed in the films confirming the theoretical predictions.

MM 69.5 Fri 10:30 H 0106

Influences of temperature and configurational disorder on electronic properties of boron carbide — •Annop Ektarawong[1], Sergei Simak[1], and Björn Alling[1,2] — [1]Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83 Linköping, Sweden — [2]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Long-standing controversial issues, concerning the electronic properties of boron carbide, are emphasized by large discrepancies between experiments and theoretical calculations. One of these is the overestimation of the bandgap of B_4C by standard DFT functionals, known to underestimate the bandgaps of all other materials. Another is the predicted metallic state of $B_{6.5}C$ in conflict with its experimental semiconducting state. With the aim of resolving such discrepancies, we investigate from first principles influences of temperature and configurational disorder, induced by low-energy defects, on electronic properties of the material. Regardless of the temperature, our results reveal a large variation in size of the bandgap and the appearance of the midgap states, both depending on the material's atomic configuration and composition, and also yield a fairly good agreement, compared to the experiments. The *ab initio* molecular dynamics simulations reveal the volumetric thermal expansion due to the lattice vibrations has a minimal impact on the bandgap of the material, while a major decrease of the bandgap is caused by explicit atomic displacements, induced by the vibrations. The temperature-dependent bandgaps of boron carbides, especially, B_4C and $B_{4.3}C$, will also be presented and discussed.